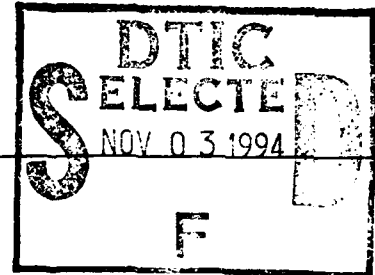


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20. Abstract

This research concerns the algorithmic development, computer implementation and direct numerical simulation of incompressible and compressible flows of naval relevance. Calculations were executed on a class of current generation multiprocessors. Pseudospectral methods were used exclusively.

Lack of parallel algorithms critical to the effective implementation of spectral methods on parallel computers necessitated the need for the development of parallel FFT algorithms for real, conjugate symmetric and real symmetric sequences. These algorithms are applied to spectral methods, but also in many areas of scientific computing. The last algorithm, the parallel fast discrete cosine transform, is used extensively in image and signal processing.

The parallel Fourier pseudospectral method for the incompressible Navier-Stokes equations was developed and implemented on many multiprocessors. Reconnection of orthogonally interacting vortex tubes was then investigated using the algorithm on parallel computers as well as vector supercomputers. Such interactions occur in turbulence, in jets and wakes, and in other strongly vortical flows. New insights into the interactions, paradigms and models were developed.

The parallel Fourier pseudospectral method for the compressible Navier-Stokes equations was also developed. Grid stretching caused aliasing errors even in linear equations. The parallelization was similar to that of incompressible flows. Shock / vortex interactions in two dimensions were investigated. Similarities and discrepancies with linear scattering theory were shown and new phenomena were observed. Compressible vortex reconnection in three dimensions was investigated by 128^3 CM simulations. Pressure signatures could not be obtained due to dynamical range considerations and the near field domain confinement. Hydroacoustic reconnection resembles that of the incompressible case. Reconnection in the high subsonic range is inhibited by compressibility effects.

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Grant N00014-89-J-1320

"Parallel Computations in Hydro-Acoustics"

Richard B. Pelz, Principal Investigator

S.G. Lekoudis, Program Manager

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Summary

This research concerns the algorithmic development, computer implementation and direct numerical simulation of incompressible and compressible flows of naval relevance. Calculations were executed on a class of current generation multiprocessors. Pseudospectral methods were used exclusively.

Lack of parallel algorithms critical to the effective implementation of spectral methods on parallel computers necessitated the need for the development of parallel FFT algorithms for real, conjugate symmetric and real symmetric sequences. These algorithms are applied to spectral methods, but also in many areas of scientific computing. The last algorithm, the parallel fast discrete cosine transform, is used extensively in image and signal processing.

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Detailed Report

The major points are underlined and appear at the beginning of each section and subsection, followed by the references.

The goal of this work is to apply massively parallel processing and spectral methods to compressible and incompressible flows that have naval applications. A Fourier pseudospectral method was used. Such methods have a very high spatial accuracy and minimal phase errors for smooth data. A number of parallel algorithms were invented stemming from their need in parallel spectral methods. Implementation was on a wide class of currently available multiprocessors.

1. Parallel FFTs

Many parallel FFT routines were developed, implemented and applied to pseudospectral methods. For a critical review of state-of-the-art methods see

Pelz, R.B., "Parallel FFTs", ICASE/LaRC Workshop on Parallel Numerical Algorithms, May 23-25, 1994, to be published.

At the heart of pseudospectral methods is the fast Fourier transform (FFT). Its discovery 30 years ago by Cooley and Tukey allowed pseudospectral methods to be competitive with finite difference and finite elements methods. In well designed pseudospectral methods codes on serial supercomputers, the majority of CPU time (about 75%) is spent executing the FFT.

Critical to an effective implementation of pseudospectral methods on parallel computers is an efficient parallel FFT. There exist two ways for computing the multidimensional FFTs needed in the methods. One is based on the rearrangement of the arrays so that the vector to be transformed is always complete within a local memory. Then a serial FFT algorithm can be used. The rearrangement is done by a parallel transposition or all-to-all personalized communication and is a global communication. This method was pioneered by the PI for pseudospectral methods in early work in this grant. The problem with this approach was that the granularity is effectively restricted to be at least the maximum sequence length. The other method, which was also applied in this project, was to keep the array layouts static and use parallel FFT algorithms. There is no restriction on granularity and with most of the multiprocessors currently available, the communication times for the block transpose and parallel FFT are the same.

1.a Application of a parallel FFTs

The minimum communication FFT algorithm was implemented, tested, extended and applied to the Fourier pseudospectral methods for the Navier-Stokes equations.

Reference Pelz, R.B. "Hypercube FFT and Fourier pseudospectral method," Parallel CFD: Implementation and Results, ed. H. Simon (MIT Press, Cambridge, 1992) pp. 189-214.

The FFT algorithm for a complex sequence which was used was that of Swarztrauber (see references in papers included). He proved that it is the minimum communication algorithm. Interestingly, there was no reference to implementation, and prior to this work, no software was written for any multiprocessor (except CM-2). The PI is currently in discussion with nCUBE for the inclusion of his FFT routines into their software library.

Upon implementation, it is found that a well-defined synchronization of processors is produced. The processor interaction and synchronization can be modeled as a nonlinear discrete

dynamical system. Steady-state solutions of the system give the synchronizations. It is found that there are multiple solutions and each are metastable. If a finite perturbation (e.g. a finite pause by one processor) is given while the processors are in one synchronization, another synchronization will be set up. Most importantly, the model yields an extremely precise form for the communication time. It also allows the pre-implementation analysis of different communication schemes, e.g., pipeline, path selection, etc.

1b Parallel FFTs for Real Sequences

Parallel FFT algorithms of sequences of real elements were invented, implemented and tested. Transforms for conjugate symmetric sequences were also developed with the new "conditional ordering".

Pelz, R.B. "Parallel Compact FFTs for Real Sequences," SIAM Journal of Scientific Computing, Vol 14, No. 4, (1993), pp.914-935.

Pelz, R.B., "A symmetric FFT for MIMD hypercubes," 5th SIAM Conference on Parallel Processing for Scientific Computing, Houston, March 25-27, 1991.

Given the general state of parallel algorithm development for scientific computation, it was reasonable to expect a lack of more specific parallel FFT algorithms. Such a transform for real input data had to be invented. FFTs of real sequences are important in spectral methods since dependent variables are real in physical space. Of course, there are numerous other applications which use it too.

Padding the imaginary part with zeros and using the parallel FFT for complex sequences (see 1a above) is wasteful in both memory and cpu time. The standard serial algorithm, due to Cooley, Lewis and Welsch, is to use pre- or post- processing to create an intermediate complex sequence of half the length and to use the complex FFT. When the sequence is distributed across processors, the processing, which is a reflection, is the worst communication possible on a hypercube (all opposite vertices of the cube must exchange data).

By taking advantage of the symmetries of the sequence at each stage of the FFT, minimum communication algorithms which have the same communication patterns as the complex one were developed. For a N length real sequence distributed evenly across P processors, $2 + \log_2 P$ nearest neighbor (hypercube) exchanges of length $N/(2P)$ are required.

For the inverse transform, which has a conjugate symmetric input sequence ($a(n) = a^*(N-n)$), parallel algorithms were developed. Key to this development was a new ordering of the input sequence. The Conditional Ordering allows the same communication structure as the complex FFT. The transform has only $1 + \log_2 P$ nearest neighbor exchanges of length $N/(2P)$.

The memory and operation count are half that of the complex FFT. The transforms are radix-2, in-place, require no extra memory and are MIMD or SIMD.

1c Parallel Cosine Transform

A parallel discrete cosine transform was invented and implemented. Applications are to symmetric Fourier methods, Chebyshev methods, and image and signal processing.

Pelz, R.B., "A Parallel, Compact FFT for Real Symmetric Sequences," proceedings of the 7th SIAM Conference on Parallel Processing for Scientific Computing, Feb 1995, San Francisco.

Pelz, R.B. "The parallel Chebyshev pseudospectral method: cosine transform and derivative recursion," Proceeding of the Fourth Conference on Hypercubes, Concurrent Computers, and Applications, (1989), pp. 433-439.

A parallel FFT algorithm for real symmetric input sequence ($a(n) = a(N-n)$) was developed. These symmetries allow expansion in a cosine series and the algorithm is also called the discrete cosine transform (DCT). The DCT is the workhorse of image and signal processing in which data compression is an important part. Historically, the DCT in this application has been limited to sequences of length 16-64 for computational expedience. Now with an efficient parallel DCT, sequence length and hence compression ratios can be increased greatly.

The parallel DCT can be applied in spectral methods when cosine and Chebyshev polynomials expansions are used. Single element domains with boundary layers can now be handled with parallel computers. Spectral element problems, in which elements are decomposed across processors and Chebyshev polynomials are used, can be implemented on parallel computers.

The serial algorithm of Cooley Lewis and Welsch uses both pre- and post-processing to create a quarter length complex sequence and coupled with a complex FFT. As in the last section, both the pre- and post-processings are reflections and require a lot of communication time.

The new parallel DCT makes use of conditional ordering as is the conjugate symmetric transform above. Using this ordering, the communication is kept to a minimum the same as the complex FFT. Making use of the symmetries during each stage, the operation count is reduced and no pre- or post-processing is needed. For an N-length sequence, $2 + \log_2 P$ nearest neighbor exchanges or 2 transposes are required. The transform is in-place, radix-2, and needs no extra memory.

2. Parallel Spectral Methods

The Fourier pseudospectral method was implemented on many multiprocessors for solving the incompressible and compressible Navier-Stokes equations. Parallel performance was asses and models developed. Suitability for scientific computational research was judged.

Pelz, R.B., "Parallel FFTs and pseudospectral methods," Physics Computing'93, Albuquerque June 1993. Invited Talk

Pelz, R.B. "Parallel Fourier spectral methods on ensemble architectures," Computer Methods in Applied Mechanics and Engineering, **89**, pp. 529-542, (1991).

Pelz, R.B. "The parallel Fourier pseudospectral method," Journal of Computational Physics, **92**, pp. 296-312, (1991).

Pelz, R.B. "Pseudospectral methods on massively parallel computers," Computer Methods in Applied Mechanics and Engineering, **80**, pp. 493-503, (1990).

Pelz, R.B. "Fourier pseudospectral method on various parallel computers," Conference of the American Physical Society, Division of Fluid Dynamics, Ithaca, NY (1990).

Pelz, R.B. "Vortex dynamics and spectral methods," Parallel CFD '89: implementation and results using MIMD computers, Los Angeles, CA (1989),.

Pelz, R.B. "Hypercube algorithms for turbulence simulation," 11th International Conference on Numerical Methods in Fluid Mechanics, Ed. D.L. Dwoyer, M.Y. Hussaini, R.G. Voigt, Lecture Notes in Physics, 323, (Springer, Berlin 1989) pp. 462-468.

Pelz, R.B. "A parallel Chebyshev pseudospectral method," Conference of the American Physical Society, Division of Fluid Dynamics, Stanford, CA (1989).

Pelz, R.B. "Parallel computations in fluid dynamics," Sixth Parallel Circus, Courant Institute of Mathematical Sciences, New York University (1989).

Pelz, R.B. "Large-scale spectral simulation of the Navier-Stokes equations on a hypercube computer," AIAA Paper 88-3642, in First National Fluid Dynamics Congress, pp. 201-206 (1988).

Pelz, R.B. "Spectral methods on hypercubes," Fourth Parallel Circus, New Brunswick, NJ (1988).

Pelz, R.B. "Spectral methods on hypercube computers," Workshop on Mathematical Aspects of Vortex Dynamics, Leesburg, VA (1988).

The parallel FFTs discussed in the previous section were used in the parallel Fourier pseudospectral method for the numerical simulation of the Navier-Stokes equations. The types of problems were vortical flows found in turbulent wakes and jets and results of the simulations will be discussed in the subsequent sections.

The goal in the present work was to investigate the performance of parallel pseudospectral methods on a variety of multiprocessors currently available. Benchmarking was performed and speedup, efficiency, parallel overhead, etc. were measured.

It is well known that development of parallel computers has been very rapid in the last few years. Changes in models, operating systems, and software have come on a monthly time scale. Benchmarking codes is like hitting a moving target. While the actual numbers that come from the tests (in the references) are most certainly out of date, the generic trends are not, thus there still is some usefulness in these publications in terms of performance.

To describe the overall algorithm, we begin by decomposing the domain, which is a cube or parallelepiped, into P equal subdomains. The number of modes or collocation points is n^3 , say. The aspect ratio of the subdomains does not effect the performance. Note that this is not the case in finite element or finite difference methods where the more cubic the subdomains are the better. If $P \leq n$ then the subdomains can be slabs, complete in two directions (coarse grain). If $n < P \leq n^2$, a 2-d decomposition is made such that the subdomains are rectangular cylinders, complete in the axial direction (medium grain). If $n^2 < P \leq n^3$ then a 3-d decomposition is made (fine grain). This decomposition holds for arrays in physical as well as spectral space.

The pseudospectral philosophy is to do derivative operations in spectral space and nonlinear ones in physical space. It can be seen that within this structure, all these operation are pointwise and require no communication. The derivative operation on a coefficient array involves a pointwise multiplication with 1-d wavenumber arrays. Typically, these arrays are global, i.e., there is a copy in each processor. Some knowledge of the processor number is then needed for the proper selection of the subarray. The fact remains, however, that the only communication is in the multidimensional FFT operation.

The first implementation was for a coarse or medium grain problem. Here the transpose method was used, in which the array decomposition was changed to make each direction complete in a sequential manner. A serial FFT algorithm was used. Because of the fact that fine grain problems could not be done with this method (e.g., 128^3 on 2048 processors) and the fact that the communication complexity of the block transpose method was the same as that of the parallel FFT, a new implementation was developed that used parallel FFTs instead of transposes. (With the advent of assembly coded serial FFTs and library-supplied transposes on some machines, the transpose may be more efficient now.)

The first implementation of the method which used parallel FFTs was done on the nCUBE and the complete code was written from scratch in FORTRAN including the FFTs. Benchmarks on the 1024 nCUBE-1 at Sandia won honorable mention in the Gordon Bell Award (see enclosed copy form IEEE Software). It was established that for 128^3 turbulence simulations, parallel computational rates rivaled those of supercomputers with assembly coded FFTs. Parallel efficiency was 80%-90%. This was quite remarkable considering the global communication needed in the FFTs.

The nCUBE code was easily portable to a class of other MIMD machines including the Intel multiprocessors. The performance on these were disappointing due to per-chip FORTRAN computational rates of 5% peak (as experienced by all researchers) as well as exceedingly large communication start-up times. Codes had to be written in i860 assembler in order to use efficiently the small cache. Current speeds on the Paragon are better.

Next the algorithm was modified for SIMD operation and ported to the CM-2. The code had to be rewritten from scratch in CMFortran (which was not a large task). On this machine, there was an parallel FFT library for complex sequences. Parallel FFT algorithms for real sequences based on the optimal serial technique were developed. It was found that the highest efficiency came from a 2-d decomposition in which the complete direction has the real to conjugate symmetric transform. This motivated the algorithm development in section 1b.

The NRL CM facility headed by Hank Dardy was used. I should like to state that this facility was run very well. I only have praise for it and their systems people.

Very good overall computational rates were obtained on the CM-2. The communication times could not be obtained and so efficiencies and communication overhead could only be inferred. The complete system, from debugging to postprocessing and storage, worked so smoothly that the NRL facility was used for the primary research work of this grant. Later, the CMs at LANL, PSC and NCSA were used.

With very little change, the codes were ported to the CM-5 and NCSA, LANL and NCAR. Another code that was developed from the incompressible one, uses complex dependent variables for complex time integration (see section 3b).

The results in this section showed that pseudospectral methods are still alive and well on parallel computers. There was serious skepticism about this fact beforehand, given the large amount of data to be communicated. The point to be remembered, however, is that spectral methods generally have more work per grid point than finite element or difference methods. This increased computation offsets the increased communication keeping the ratio between the two favorable. Spectral methods also tend to minimize the number of grid points and hence memory. The lower amount of memory for the same accuracy allows for reduced amount of data to be communicated.

3. Applications in Incompressible Flows

The starting point for performing fluid dynamic research on parallel computers was to do some outstanding and important problems in incompressible flows.

3a. Incompressible Vortex Reconnection

256³ direct simulations were made on the CM-2 of vortex reconnection. The dynamics were explained; models and the link to turbulence were made

Boratav, O.N., Pelz, R. B. and Zabusky, N. J. "Reconnection in orthogonally interacting vortex tubes: Direct numerical simulations and quantifications," The Physics of Fluids A, 4 (1992).

Boratav, O.N., Pelz, R. B. and Zabusky, N. J. "On vortex reconnection and turbulence," in Topological Aspects of the Dynamics of Fluids and Plasmas, Moffat, Zaslavsky, Comte and Tabor eds., NATO ASI Series, (Kluwer, Dordrecht), 1992, pp.363-376.

Zabusky, N.J., Boratav, O.N., Pelz, R.B., Gao, M., Silver, D. and Cooper, S., "Emergence of coherent patterns of vortex stretching during reconnection: A scattering paradigm," Physical Review Letters, 67 n 18, pp.2469 (1991).

Boratav, O.N., Pelz, R. B. and Zabusky, N. J. "Winding and reconnection mechanisms of closely interacting vortex tubes in three dimensions," in Vortex Dynamics and Vortex Methods, Greengard & Anderson eds., American Mathematical Society (AMS), Lectures in Applied Mathematics, Vol.28, (1991).

Pelz, R.B., "Vortex dynamics and turbulence on ensemble architectures," 2nd International Conference on Industrial and Applied Mathematics, Washington, DC, July 8-12, 1991.

Boratav, O, Pelz, R.B., Silver, D and Zabusky, N, "Collapse and reconnection of orthogonally offset vortex tubes in three dimensions," 2nd International Conference on Industrial and Applied Mathematics, Washington, DC, July 8-12, 1991.

O. N. Boratav, R. B. Pelz and N. J. Zabusky, "Evolution During Reconnection of the Strain Rate, Velocity Gradient Tensor Invariants," Conference of the American Physical Society, Division of Fluid Dynamics, Scotsdale, AR (1991).

R. B. Pelz, O. N. Boratav and N. J. Zabusky, "Fingering Mechanisms of Closely Interacting Vortex Tubes in Three Dimensions," Conference of the American Physical Society, Division of Fluid Dynamics, Scotsdale, AR (1991).

N. J. Zabusky, O. N. Boratav, R. B. Pelz, M. Gao, S. Cooper, and D. Silver, "Emergence of Coherent Patterns of Vortex Stretching During Reconnection," Conference of the American Physical Society, Division of Fluid Dynamics, Scotsdale, AR (1991).

S. Cooper, N. J. Zabusky, D. Silver, M. Gao, R. B. Pelz, O. N. Boratav and R. Samtaney, "Space-Time Diagrams and Volumes: Projections of Thresholded Functions for Visualizing and Quantifying 2D and 3D Evolving Phenomena," Conference of the American Physical Society, Division of Fluid Dynamics, Scotsdale, AR (1991).

Boratav, O.N., Pelz, R.B., Zabusky, N.J., Silver, D. and Cooper, S.P., Cover Photograph of Computers in Physics, Nov/Dec Vol 4, No 6 (1990).

Pelz, R.B., Boratav, O., Zabusky, N., Silver, D. and Gu., "What happens when two vortexes (sic) meet?" (editor's title) Visualization News Interview in Pixel, July/Aug, 3 1990.

Pelz, R.B. "Vortex Reconnection," International Symposium on Structures in Continuous Media, USSR, June 11-20, 1990, Invited Talk.

Boratav, O., Pelz, R. and Zabusky, N. "Vortex scattering and reconnection: numerical simulation of closely interacting vortex tubes," Conference of the American Physical Society, Division of Fluid Dynamics, Ithaca, NY (1990).

Boratav, O.N., Pelz, R.B., Zabusky, N.J., Silver, D., Cooper, S.P., Appino, P.A., Liu, C.N. Rabenhorst, D.A. and Depillis, J., "Bursting Reconnection of Closely Interacting Vortices in Three Dimensions," Video entry in Gallery of Fluid Motion, Conference of the American Physical Society, Division of Fluid Dynamics, Ithaca, NY (1990).

Boratav, O.N., Pelz, R.B., Zabusky, N.J., Silver, D. and Cooper, S.P., "Vortex 'Plowing' and Counter-Helical Winding of Closely Interacting Vortex Tubes in Three Dimensions," Video entry in Gallery of Fluid Motion, Conference of the American Physical Society, Division of Fluid Dynamics, Ithaca, NY (1990).

Boratav, O., Pelz, R., Zabusky, N. & Liu, S. "Asymmetric vortex reconnection," Video entry in: Gallery of Fluid Motion, Conference of the American Physical Society, Division of Fluid Dynamics, Stanford, CA (1989).

Boratav, O., Pelz, R., Zabusky, N., Silver, D. & Gu, S. "New morphologies in asymmetric vortex reconnection," Poster in: Gallery of Fluid Motion, Conference of the American Physical Society, Division of Fluid Dynamics, Stanford, CA (1989).

Turbulent and complex flows in jets and ship wakes contain regions of high vorticity. Understanding the dynamics of interacting vortical regions in both incompressible and compressible flows may lead to the development of detection methods and bodies which minimize such interactions. Because of this, the first application for pseudospectral methods on parallel computers was the simulation of the close interaction of vortex tubes.

This project, in which the low resolution runs were done on vector supercomputers and the high resolution ones on parallel computers, was done in collaboration with N. Zabusky and formed the Ph.D. thesis on O. Boratav. The incompressible runs were needed to compare to the compressible ones.

The CM-2 runs at resolutions up to 256^3 were done at the NRL facility. At the time these were the highest resolution ever done in direct spectral simulations. The flows were analyzed in detailed, which was difficult given the amount of data. The CM-2 facility allowed post processing and manipulation fairly easily.

There has been numerous studies of vortex reconnection, particularly with the Crow instability initial conditions of perturbed antiparallel vortex tubes. We found that a more generic initial condition, the orthogonal offset arrangement, offered a richer dynamics and a larger parameter space in which to explore.

When orthogonal vortex tubes are close to each other, they attract and contort so that a segment of the tubes has a nearly antiparallel alignment. During this process, small but strong pieces of the main tubes (hairpins) are pulled off and stretched in the strain fields. We termed this *fingering* and is an important generation mechanism for small scale vorticity. (see Kida's paper in 1994 Annual Review of Fluid Mechanics)

The antiparallel tube segments then collapse due to the nonlocal strain generated by the complement parts of the tubes. The collapse is violent and is a function of viscosity and initial circulation. We developed a model of reconnection. In the center between collapsing tubes, the leading vortex lines pinch at a so called X point. Because of the rapid change in vorticity, viscous diffusion is high and the line vortex concepts (Helmholtz's theorem) do not hold. The vortex vector field is disjoint. Viscous dissipation quickly diminishes the strength of the vorticity in the tube direction.

The vortex dipole has two stagnation points, the upper (head) has a positive rate of strain in the direction orthogonal to the tube and the induced velocity. Because the tubes pinch, there is also vorticity in this direction which is positive on one side of the pinch of both tubes and negative on the other side. Viscous diffusion acting on this even function of vorticity, tends to level it out. The strain field around the head stagnation point quickly increases the vorticity.

The curvature in the growing orthogonal vorticity field is high. Self-induced motion causes a reduction of curvature and a movement away from the high dissipation region. As the line vortex concept becomes applicable again, the observation is that the vorticity vectors have "reconnected" in the orthogonal direction. The vortex lines in one tube run into the other tube and vice-versa.

The nonlocal strain responsible for the collapse forces more vortex lines into the dissipation region and to reconnection. As the strength of the newly formed tubes increases, a new strain counteracts the original and halts the collapse. The new tubes move away from the interaction region to further reduce curvature.

Reconnection of all the lines in the original tubes may not occur, and a rather inert remnant of vorticity is left in the interaction region. The completeness of the interaction is a function Reynolds number and individual initial strengths.

A model of this interaction as a scattering at an X point was proposed and an analysis of the normalized vortex stretching vector yielded closed loop field lines during the interaction. Forming a halo around the X point / pinch region, the stretching diminished the original vorticity and increased the newly formed vorticity. The bridges or bulges in vorticity which are always seen in reconnection occur at the head stagnation point of the dipole and run through the stretching halo.

A detailed analysis was done on the connection between reconnection and turbulence. In particular, the behavior of the rate of strain tensor and vorticity vectors was studied. During the interaction, the statistics of the alignment and magnitude of the rate of strain eigenvectors and vorticity show striking similarities with that of fully developed turbulence. The energy spectrum is much steeper than in turbulence, however.

The vortex tube interaction has been proposed as possibly leading to a finite-time singularity of the incompressible Euler equations. We studied this problem for various Reynolds numbers using various norms of vorticity and dissipation rate. While actual interaction rate models were not developed, models proposed by others were shown to be incorrect.

Reconnection was found to increase greatly the total helicity (a constant in inviscid flow). This is caused not by the actual reconnection of the tubes, but the twistedness of the vortex tubes in the interaction. A measure of this is the vorticity, $\omega \times \nabla \times \omega$, or the helicity of the vorticity vector.

3b Turbulence Simulations in Complex Time

The 128³ CM simulations of homogeneous turbulence were made in complex time to explore the singularities which effect real time dynamics.

Kimura, Y. and Pelz, R.B., "Search for Complex Time Singularities in Navier Stokes Turbulence," in Unstable and Turbulence Motion of Fluid, eds. S. Kida (World Scientific, Singapore) 1994, pp. 91-101.

Kimura, Y. and Pelz, R.B., "Turbulence Simulations in Complex Time," Workshop on Mathematical Aspects of Turbulence, Kyoto September 1992.

An exciting new application of parallel spectral methods is the simulation of isotropic homogeneous turbulence in complex time. The incompressible Navier-Stokes equations are analytically continued into the complex time domain. All dependent variables become complex and the number of independent variable are 5, thus putting addition strain on computational resources. Integration then occurs along a parameterized curve in the complex time domain.

The reason for this study is to search for and classify singularities in the complex plane which influence significantly the real time dynamics. Real time phenomena can be viewed as a result of nearby singularities in complex space time. The exponential scaling factor on k in the energy spectra is related to the distance of the nearest singularity to the real plane. If the local and functional form of the closest singularities can be found, a reduced model, containing just this information, can be constructed. It is expected that these singularities are isolated and are poles of noninteger order.

As a first step towards this goal, the enstrophy and energy spectra were mapped out in the complex time plane below singularities using the CM-2. Further unpublished work done on the CM-5 revealed a rich structure of singularities which could not be deduced by the real time dynamics. Their distribution is a function of Reynolds number and initial field. Many are observed after the peak in enstrophy and well into the decay period of the unforced turbulence. Further publications will acknowledge this grant.

4. Compressible Flow Calculations

4a. The Compressible flow Code

We developed the parallel algorithm and wrote a Fourier pseudospectral method code on the CM for performing simulations of the 2-D and 3-D unsteady, viscous, compressible Navier-Stokes equations.

A periodic box served as the computational domain. It was chosen because of its simplicity and because the mechanisms in the interior are of interest and not interactions with boundaries. A one-dimensional version was written to get fast results for plane wave propagation cases. As with the algorithm for incompressible flow, the multidimensional FFT was the only operation which required communication.

Three different time stepping schemes were compared in order to minimize the overall CPU time for a certain real time simulation: Second-order Adams-Bashforth with third- and fourth-order low-storage Runge-Kutta algorithms. Such an optimization is important since the Courant number limits the maximum time step severely. The comparisons showed that it is advantageous to use the fourth-order RK algorithm, even if it requires four times as much work per time step as for example the Adams-Bashforth scheme. RK4 remains stable with a much larger time step and the overall CPU time can therefore be reduced by a factor of three in our parameter range.

Tests with a time-split scheme, where the acoustical terms are integrated analytically, were not convincing. (This scheme is used by Erlebacher, Hussaini, et al.) The idea of being able to increase the maximum allowable time step by a considerable amount could not be realized at even moderate Mach numbers. Therefore, the originally proposed Runge-Kutta scheme was implemented for the time integration.

The code validation was done by running simple test cases and then by comparing them with known analytical results. Weak acoustic waves were set up and the speed of propagation was checked. Simple elements (acoustic monopoles and dipoles) were initialized and the invariance with respect to rotation and the directivity patterns were examined. For stronger sources steepening of the wave front as a function of the Reynolds and Mach numbers was tested. The results exposed an often neglected phenomenon that even weak nonlinearities are cumulative unless the Reynolds number is very low.

The compressible Navier-Stokes code developed allows a detailed simulation of the near field and zone of interaction. Such information cannot be obtained by the standard methods of analytical acoustics, which give generally far field solutions in the asymptotic limit. We were able to examine in detail the interaction of variable-strength sound waves and fluid flows.

4b. Wave/Vortex Simulations

The interaction of shock and acoustic waves on a planar vortex is studied numerically. Mach number, vortex width and wave form formed the parameter space. Similarities and deviations from linear theory are discussed.

Scheidegger, T. and Pelz, R., "Acoustic wave / vortex interaction," Conference of the American Physical Society, Division of Fluid Dynamics, Ithaca, NY (1990).

One of the main new phenomena encountered in compressible turbulence (as opposed to incompressible turbulence) is the interaction of sound waves and vortices (eddies, coherent structures). Direct simulations of compressible turbulence are topologically too complex to resolve such single events. We need to understand isolated wave/vortex interactions before tackling compressible turbulence.

Our initial conditions were relatively simple and very deterministic. A compressible wave interacts orthogonally with a columnar vortex. This configuration was chosen because it allowed the time and length scales to be set apriori. It also allowed us to separate initially the compressible flow part from the underlying solenoidal field. This latter point proved to be very important in our simulations. We found that if the initial flow field does not satisfy the governing equations, artificial compressibility builds up in a very short time and obscures the actual interaction process.

A difficulty encountered was the low convergence rate of our Fourier spectral method for nonsmooth data. Low-pass filters were used in addition to lower Reynolds numbers in order to weaken the discontinuities of forming shock waves. The simulations showed that too much

viscosity leads to aeroacoustic radiation due to the viscous decay of the vortex. Therefore, we controlled the high wavenumber modes solely by repeated filtering of the field variables with no extra viscosity. A filter with exponential characteristic at higher modes showed good results. It was found that it is sufficient in aeroacoustic computations to filter only the compressible modes if the vortical flow is initially smooth enough. Different vortex velocity profiles were compared for this reason. The actual velocity distribution was not very crucial for the interaction. All our later experiments were performed with a Taylor vortex which has a linear varying angular velocity in the core and an exponential decay outside.

The physically relevant parameters of the interaction problem are primarily the vortex length scale, the vortex Mach number, the incident wavelength and the wave strength. We varied the maximum Mach number of the vortex from 0.1 to 1.1. Among the incident wave was a Gaussian profile with fixed standard deviation. The vortex core dimensions were varied in order to investigate the influence of the incident wavelength. Ratios of core size to pulse width were obtained between 0.2 and 20.

After careful analysis it was found that an important parameter is the ratio λ/l between incident wave length and vortex diameter. Backscattering in the strict sense was very small for all ratios. But it was found that the long wavelength limit is already reached for $\lambda/l=2.5$ and that scattering at ± 45 degrees with respect to the backward direction is as important as forward scattering. The whole vortex acts as a simple quadrupole, independent of the actual core structure. This result indicates the limitations of parabolic approximations for the wave equation if the dominant length scales are small compared to the incident wave.

The results differ significantly depending on the vortex strength. We found at low Mach numbers qualitative agreement with linear theory in the sense that scattering occurs dominantly in the forward direction and that density inhomogeneities are not important scatterers. Backscattering is almost negligible. The amplitude functions of the scattered signal show maxima at angles from the direction of the incident wave between 25 and 40 degrees. The angle increases with decreasing ratio of core size to wave length. The wave strength does not affect the directivity pattern. The directivity pattern and maxima, which cannot be predicted from linear theory, are important and new results of our study.

Some literature in turbulence reports a rather abrupt change in behavior of the compressible mode at a certain Mach number depending on the initial compressibility. We found a gradual change in the results with increasing Mach number. An interaction at $Ma=0.8$ is far beyond the limits of a classical scattering theory. Nonlinear convection of the sound and acoustic vortex instability become important.

A detailed examination of the vortex core during the interaction revealed that a counter rotating spiral wave, generated at higher Mach numbers, exists and can be attributed to the convection and acceleration of core vorticity. The net energy transfer from the solenoidal to the compressible mode was measured. For $Ma < 0.3$ there is no increase in compressible energy detectable. This changes with increased vortex strength. For $Ma=0.9$ the increase is 5% after one interaction.

In order to understand the wave/vortex interaction, the process was analyzed by decomposing the velocity field into its compressible and solenoidal modes and by evaluating the time dependent quadrupole source terms in Lighthill's equation. This velocity decomposition allowed us to differentiate between the sources which cause aerodynamic noise, scattering noise and nonlinear self-interaction. The strong forward scattering results at low Mach numbers can clearly be recognized in the dominant longitudinal quadrupoles in the direction of the incident wave. At higher vortex strength the same quadrupole dominates initially, but the lateral poles

gain very shortly afterwards and this leads to the more complex wave pattern. Strong vorticity distributions enhance isotropy in the compressible energy spectrum.

Monochromatic wave scattering was simulated in order to compare the scattering amplitudes qualitatively with analytical expressions (first Born approximation). The measured amplitude functions agree well with the theory for low Mach numbers. The deviations are less than 5% at the angle of maximum scattering for $\lambda/l=2$. It is of practical interest that the theory predicts, despite its assumptions, good results even for wavelengths comparable in size with the vortex length. The good agreement between simulations and theory also indicates that the far field limit is reached within a small number of wavelengths from the sound sources.

Two discrepancies between the numerical simulation and theory were found. The scattering amplitude function is shifted downwards and in the direction of the vortex motion. The first shift is caused by the uniform diffraction due to symmetrical density inhomogeneities. The latter can be explained by the convection of sound by the underlying flow field. Both phenomena are neglected in the Born approximation. The angular shift amounts to more than 5 degrees for $Ma > 0.2$.

4c. Grid Stretching

Another result which we have obtained from observation of our simulations may have serious ramifications for spectral methods. We were attempting to observe the shock/vortex interaction and subsequent evolution as an isolated event, free from boundary conditions. In order to accomplish, we employed a smooth mapping to stretch the outer parts of the domain. Encountering unphysical results, we analyzed two model problems, the 1-D Berger's equation and 1-D linear advection equation, on a stretched grid. A wave packet initial condition was propagated in time using the linear advection equation. As the packet approaches the edge of the fine mesh, large oscillations appear on the other side of the fine mesh, small-scale oscillations appear throughout the fine grid and the packet is not propagated at the correct wave speed on the course grid. This is an unexpected result especially for the linear equation in which no aliasing occurs. This example points to a possible serious drawback to using spectral methods on stretched grids, a common procedure for boundary layer flows.

4d. Compressible Vortex Reconnection

Simulations of orthogonally offset vortices in compressible flow suggest that in the hydroacoustic limit, reconnection is similar to the incompressible case and that an increase in compressibility leads to an inhibition of reconnection.

R.B. Pelz, T.Scheidegger, and N. Zabusky, "Compressible Vortex Reconnection on the Connection Machine," Parallel CFD'92, eds. Pelz, Ecer, Häuser, (North-Holland, Amsterdam) 1993 pp.

We performed direct numerical simulations of compressible fluid flows on the Connection Machine. The compressible flow DNS, 128^3 , was performed on the CM2. The initial condition was orthogonal offset vortex tubes. The significance of such a configuration in the view of numerical aero-acoustics is that the scale separation between acoustic wave length and flow structure can be large, depending on the Mach number. This stands in contrast to the scattering simulations above with imposed scales. The vortex interaction problem is, therefore, an important testbed to check the feasibility of computational aero-acoustics. It shows whether both scales can properly be resolved. In addition to providing insight into the fundamental mechanisms of sound generation by flow fields, it also relates to compressible turbulence.

The simulations performed covered Reynolds numbers between 1300 and 3900, with Mach numbers ranging from 0.45 to 0.95. For low Ma, the overall features compare qualitatively well with incompressible results of the same initial configuration. Both vortex tubes approach each other, form a local dipole, and then reconnect very rapidly. After this sudden change in topology, both vortices move away without any further interaction. It is found that many variables -such as vorticity, divergence, and strain rate are amplified by a large amount. This amplification is very local and located around the center of the dipole.

The reconnection mechanism was investigated with respect to sound generation. It was found that, for the covered parameter range, no significant increase in radiation can be measured directly by monitoring pressure fluctuations. An analysis of the sound sources (unsteady Lighthill stresses) showed two activity peaks during the evolution. A considerable amount of background noise is caused in a fast transition period at the beginning of the simulations. The actual reconnection process leads to source amplifications of $O(10)$. However, these sources cover a much smaller portion of the flow than the ones generated during the initial relaxation. Consequently, the feasibility of measuring directly the sound emission of isolated flow structures depends on the ability to set up sufficiently quiescent initial conditions.

A scheme based on the acoustic analogy was created to extrapolate the far field pressure. It uses source information obtained from the computations and includes retarded time effects. A verification in 3D is difficult since the whole numerical domain lies in the near field and no experimental data are available for comparison. The scheme has been validated for simple 1D cases.

We have observed critical differences in this event due to compressibility. As the Mach number is raised through the high subsonic range, the whole process of reconnection changes. No longer is there an X-point, but a double Y and reconnection times are longer. In the center of the dipole, the flow accelerates to supersonic speeds. A normal shock forms towards the head of the vortex. This effect causes the vortices to halt their collapse. They do not pinch but the rather the dipolar region remains extended and two-dimensional. At the end of the dipole region (Y points), reconnection of some vorticity takes place but at a slow rate. Gradient quantities such as dissipation rate do not rise significantly as they did in incompressible flow. This is not in the hydroacoustic range, unfortunately, but is in the aeroacoustic range and may have applications to jet noise.